ELEMENTS OF DETONATION THEORY (HIGH-SPEED COMBUSTION)

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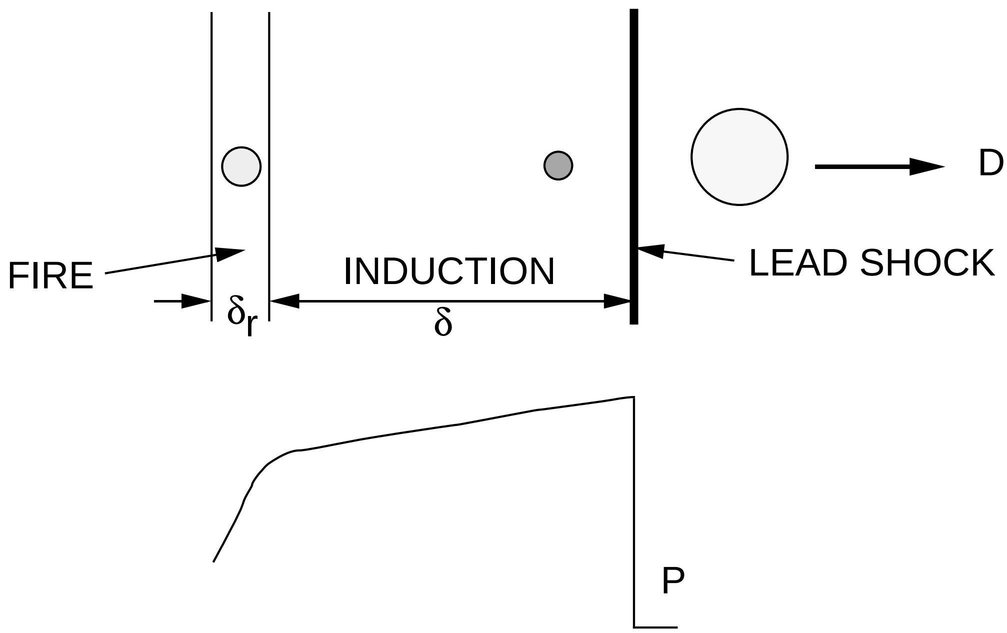
HIGH-SPEED ENVIRONMENT

- Nonpremixed Combustion
  - high speed shear layers
    (hypersonic air-breathing propulsion)
- **Premixed Combustion**
  - **fast flames** (subsonic)
  - **detonations** (supersonic)

<u>Detonations</u>



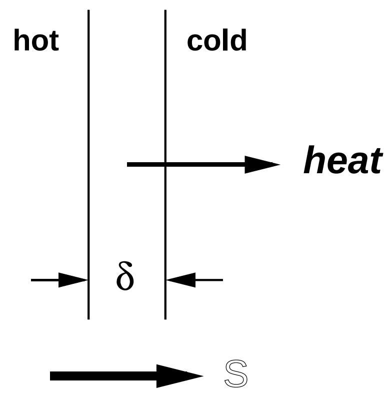
Propagation via autoignition caused by shock compression
Rapid, violent, spectacular

$$D \sim \sqrt{q} \sim 2000 \text{ m/s in gases}, \quad q : \text{specific chemical energy}$$

Power density (high explosives) $\sim 10^{10}$ watt/cm ^{2}

ZND structure (shock followed by fast flame)

Deflagrations



Thermal diffusivity $\alpha \sim 10^{-5}$ m^2 s^{-1}
Chemical time $t_c \sim 10^{-3}$ s

$$S \sim \sqrt{\frac{\alpha}{t_c}}, \quad \delta \sim \sqrt{\alpha t_c}$$

$$S \sim \text{cm/s}, \quad \delta < 1\text{mm}, \quad \frac{\Delta p}{p} \ll 1$$

Slow, subsonic, nearly-isobaric, diffusion-controlled

Power density $\sim 10^2$ watt/cm^2

Study of Detonations

Practical Motivation

- Wanted detonations: accurate prediction of behavior in usage
- Unwanted detonations: safety issues in transport, storage and handling

Status of Theory

- Steady structure is generally well-understood
- Unsteady behavior less so and requires further work
  - evolution from quiescent conditions upon stimulus
  - transition from deflagration to detonation (DDT)
  - instabilities: development of cellular structures
  - failure to propagate
- Difficulties in modelling due to
  - **Mechanical and chemical complexity of explosive media**
  - **Lack of detailed observational data**
- **Heterogeneous explosives are particularly challenging**

A Basic Model (gaseous reactants)

- Diffusion plays a negligible role in fast flames
  - u, particle speed
  - c, sound speed ($\sim$ molecular speed)
  - t_{coll}, collision time
  - ν, kinematic viscosity ($\sim c^2 t_{\text{coll}}$)
  - L, characteristic length
  - t_{chem}, chemical time $\gg t_{\text{coll}}$
  - dimensionless parameters
    * $M = u/c$, Mach number
    * $Re = uL/\nu$, Reynolds number
    * $\mathcal{D} = L/u\, t_{\text{chem}}$, Damköhler number

  Significant chemical-flow coupling

  $\Rightarrow \mathcal{D} = O(1) \quad \Rightarrow L \sim u t_{\text{chem}}$
  $\Rightarrow Re \sim u^2 t_{\text{chem}}/\nu \sim M^2 t_{\text{chem}} c^2/\nu \sim M^2 t_{\text{chem}}/t_{\text{coll}}$
  $M = O(1) \Rightarrow$

  $Re \gg 1$

  (In flames, $M \ll 1 \Rightarrow Re$ moderate)

- Inertial confinement (constraint on expansion)

  $L \sim u\, t_{\text{chem}} \sim c\, t_{\text{chem}}$
  - substantial chemico-acoustic interaction
  - significant pressure rise (in contrast to flames)

Basic Model, contd.

Balance Laws

mass:	$\dot{\rho} + \rho \nabla \cdot \mathbf{u} = 0$
momentum:	$\rho \dot{\mathbf{u}} + \nabla p = 0$
energy:	$\dot{e} + p \dot{v} = 0$

$$\dot{f} \equiv \frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f$$

Constitutive Assumptions

- exothermic kinetics $\mathcal{A} \Longrightarrow \mathcal{B}$
- progress variable λ, $0 \leq \lambda \leq 1$
- rate law

$$\begin{aligned} \dot{\lambda} &= \mathcal{R}(p, v, \lambda) \\ &= (1-\lambda)^s K(p, v) \\ &= k(1-\lambda)^s \exp(-T_a/T) \end{aligned}$$

- equation of state

$$e = e(p, v, \lambda) = \frac{pv}{\gamma - 1} - \lambda q, \quad q = \text{ heat of reaction per unit mass}$$

γ = adiabatic exponent, logarithmic slope of isentrope

$1 < \gamma < 2$ for gases

$\gamma > 2$ mimics condensed materials (stiffer than gases)

Constitutive Assumptions, contd.

- Ideal material

$$pv = RT$$

- sound speed

$$c = \sqrt{\gamma p v}$$

Caveats

- **Typically, kinetics is complex (multiple reactions and species, mole change, endothermic steps)**
- **Mixture equations of state (especially for condensed explosives) are difficult to characterize and are a subject of active research**

Basic Model (Reactive Euler Equations), planar, contd.

Conservative form

$$\begin{aligned}
\rho_t + (\rho u)_x &= 0 \\
(\rho u)_t + (p + \rho u^2)_x &= 0 \\
(\rho E)_t + [\rho u(E + pv)]_x &= 0 \\
(\rho\lambda)_t + (\rho u\lambda)_x &= \rho\mathcal{R}
\end{aligned}$$

$$\begin{aligned}
E &= e + \frac{1}{2}u^2, \quad \text{total energy per unit mass} \\
e &= \frac{pv}{\gamma - 1} - \lambda q, \quad \text{internal energy per unit mass}
\end{aligned}$$

Alternate (nonconservative) form

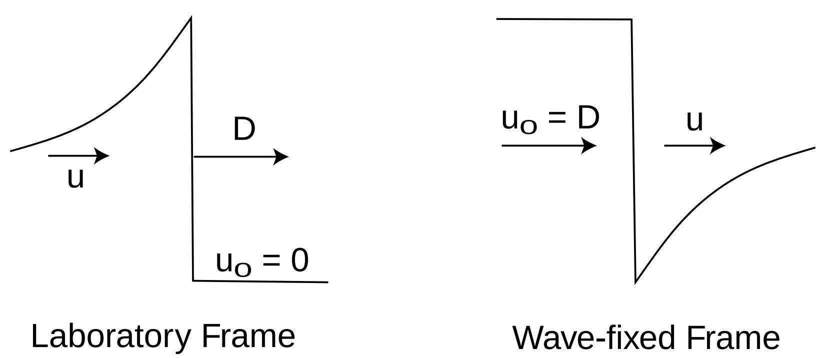
$$\begin{aligned}
\dot{\rho} + \rho u_x &= 0 \\
\dot{u} + v p_x &= 0 \\
\dot{p} + \rho c^2 u_x &= \frac{\gamma - 1}{v}(q\dot{\lambda}) \\
\dot{\lambda} &= \mathcal{R}
\end{aligned}$$

Characteristic form (hyperbolic system)

$$\begin{aligned}
\left(\frac{dp}{dt}\right)_\pm \pm \left(\frac{d\rho}{dt}\right)_\pm &= \frac{\gamma - 1}{v} q\mathcal{R}, \qquad \left(\frac{dx}{dt}\right)_\pm = u \pm c \\
\dot{p} - c^2\dot{\rho} &= \frac{\gamma - 1}{v} q\mathcal{R} \\
\dot{\lambda} &= \mathcal{R}, \qquad \left(\frac{dx}{dt}\right)_\pm = u
\end{aligned}$$

Steady Travelling Waves

- For a given ambient state, and a **given wave speed D**, the steady theory determines the feasible end states and structure
- Relating the wave speed to the ambient requires other considerations



State upstream(wave-fixed frame)

$$p_0,\ v_0(=1/\rho_0),\ u_0(=D),\ \lambda_0(=0)$$

State within

$$p,\ v(=1/\rho),\ u,\ \lambda$$

Steady Travelling Waves, contd.

Conservation relations

$$\rho_0 D = \rho u$$

$$p_0 + \rho_0 D^2 = p + \rho u^2$$

$$e(p_0, v_0, 0) + p_0 v_0 + \frac{1}{2}D^2 = e(p, v, \lambda) + pv + \frac{1}{2}u^2$$

Rayleigh line

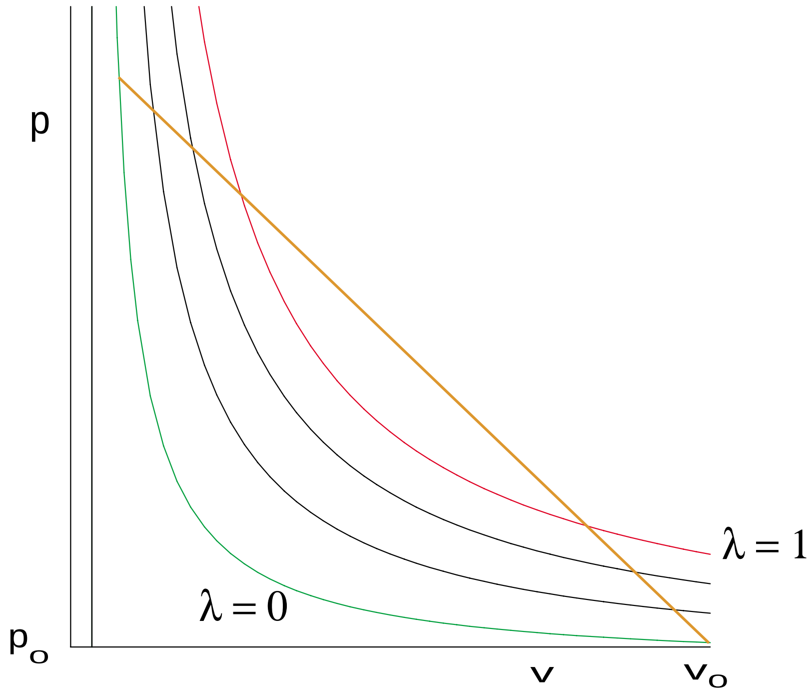
$$p - p_0 = -\rho_0^2 D^2 (v - v_0)$$

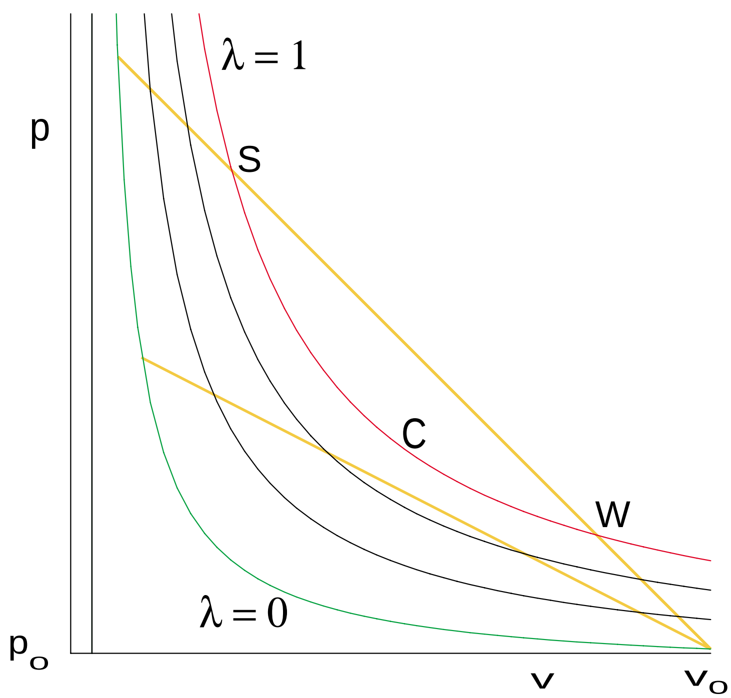
Hugoniot Curve

$$e(p, v, \lambda) - e(p_0, v_0, 0) = \frac{1}{2}(p + p_0)(v_0 - v)$$

Hugoniot for the ideal material,

$$\left(\frac{p}{p_0} + \Gamma\right)\left(\frac{v}{v_0} - \Gamma\right) = 1 - \Gamma^2 + 2\Gamma\frac{\lambda q}{p_0 v_0}; \quad \Gamma = \frac{\gamma - 1}{\gamma + 1} > 0$$


p
p_o
$\lambda = 1$
$\lambda = 0$
v
v_o


p
p_o
$\lambda = 1$
S
C
W
$\lambda = 0$
v
v_o

Steady Travelling Waves, contd.

Scaled Quantities

$$U = \frac{u}{D}, \quad V = \frac{v}{v_0}, \quad P = \frac{p}{\rho_0 D^2}, \quad Q = \frac{q}{D^2}$$

Conservation Conditions

$$U = V$$

$$P = P_0 + 1 - V$$

$$(P + \Gamma P_0)(V - \Gamma) = (1 - \Gamma^2)P_0 + 2\Gamma\lambda Q$$

Wave Structure (function of λ, for given D)

$$P = \frac{1 + P_0 \mp S}{\gamma + 1}$$

$$V = U = \frac{\gamma(1 + P_0) \pm S}{\gamma + 1}$$

$$S = [(1 - \gamma P_0)^2 - 2\lambda Q(\gamma^2 - 1)]^{1/2}$$

Steady Travelling Waves, contd.

Simplified wave structure, $P_0 \ll 1$

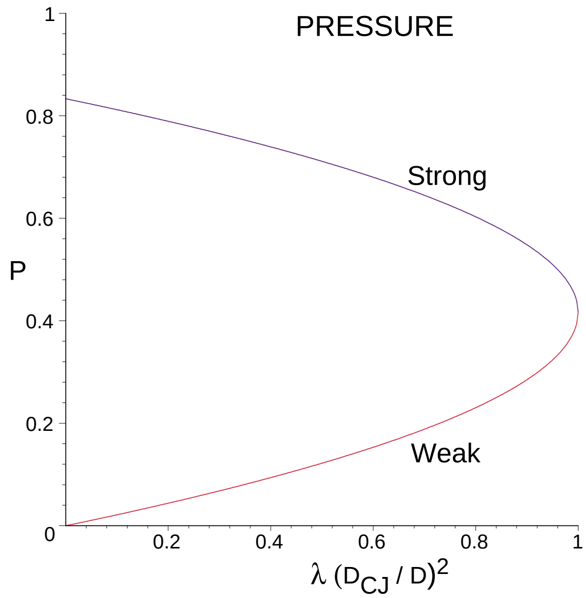
$$
\begin{aligned}
P &= \frac{1 \mp S}{\gamma + 1} \\
V &= U = \frac{\gamma \pm S}{\gamma + 1} \\
M &= \sqrt{\frac{U^2}{\gamma P V}} = \sqrt{\frac{1 \pm S/\gamma}{1 \mp S}} \quad \text{(Mach number)} \\
S(\lambda; D) &= [1 - 2\lambda Q(\gamma^2 - 1)]^{1/2}, \quad Q = q/D^2
\end{aligned}
$$

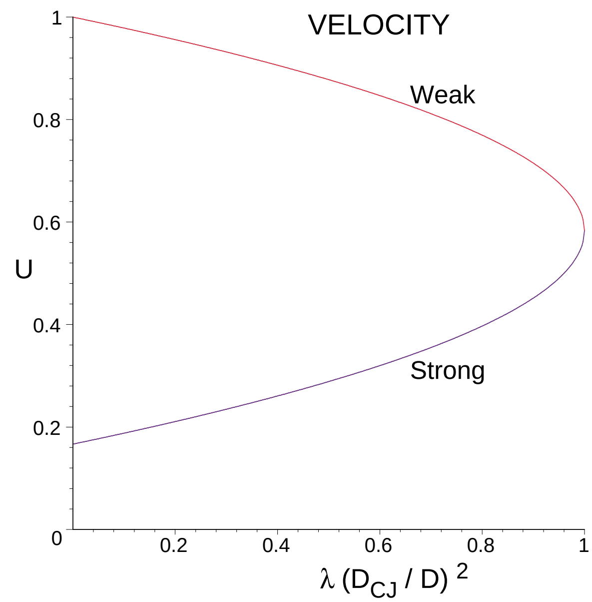
- $S(1; D)$ real $\Rightarrow$

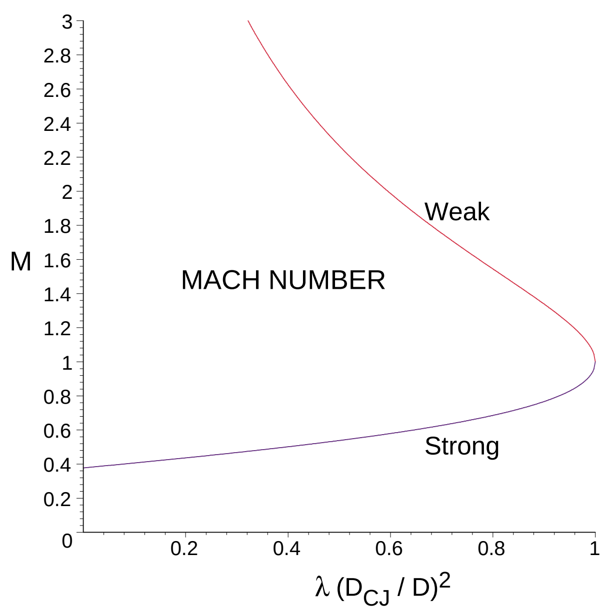
$$D \geq D_{CJ} = \sqrt{2q(\gamma^2 - 1)}$$

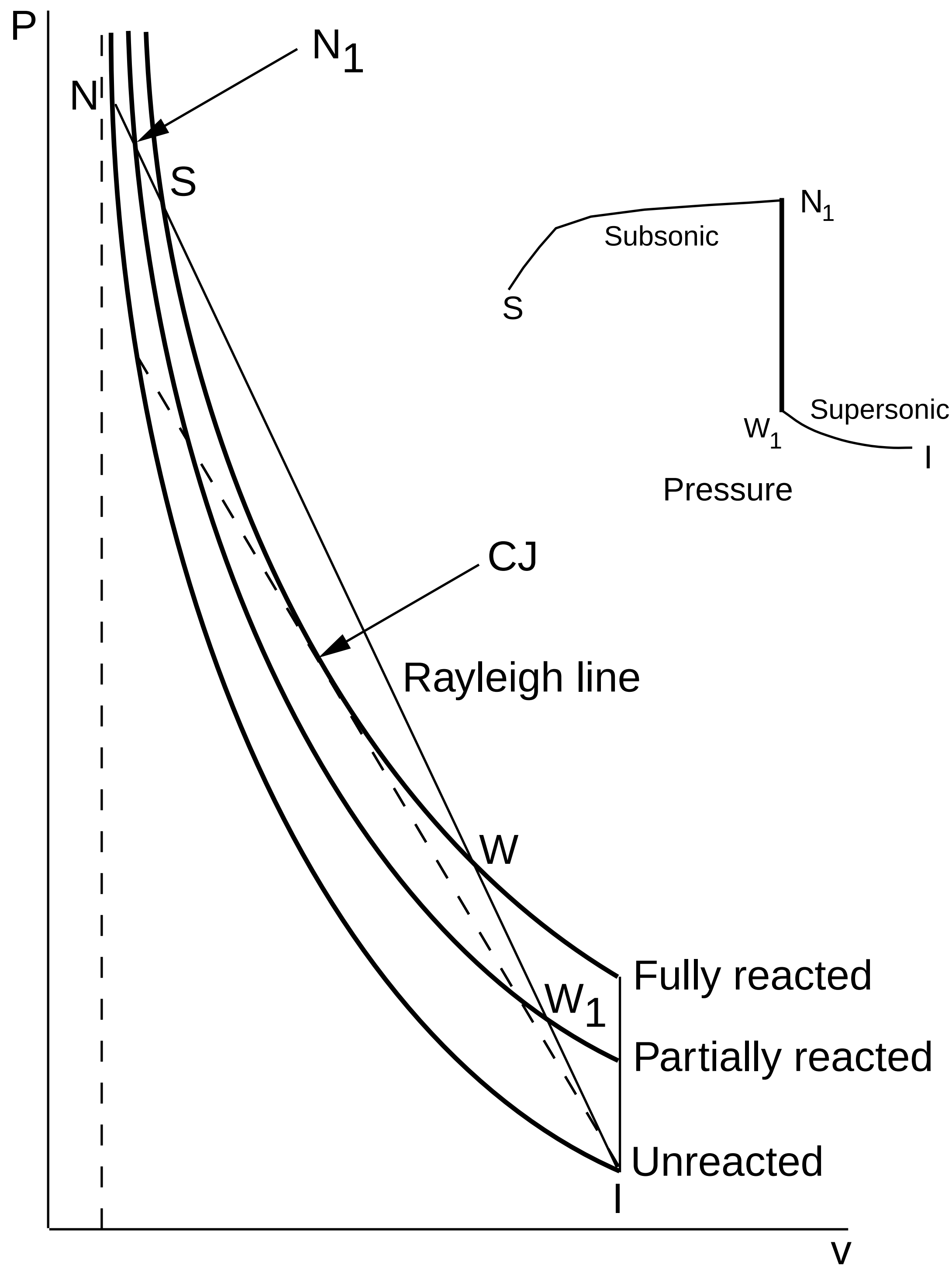
$$S(\lambda; D) = [1 - \lambda\, D_{CJ}^2/D^2]^{1/2}$$

- Solution has two branches
- Upper sign supersonic, lower subsonic
- $S(0; D) = 1 \ \Rightarrow$ solution with upper sign limits to upstream state $(P = 0)$ at $\lambda = 0$
- Lower sign corresponds to a jump (shock) at $\lambda = 0$


PRESSURE
P
Strong
Weak
0
0.2
0.4
0.6
0.8
1
λ (D_CJ / D)^2


VELOCITY
U
Weak
Strong
0
0.2
0.4
0.6
0.8
1
λ (D_CJ / D) 2


MACH NUMBER
M
Weak
Strong
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
λ (D_CJ / D)^2

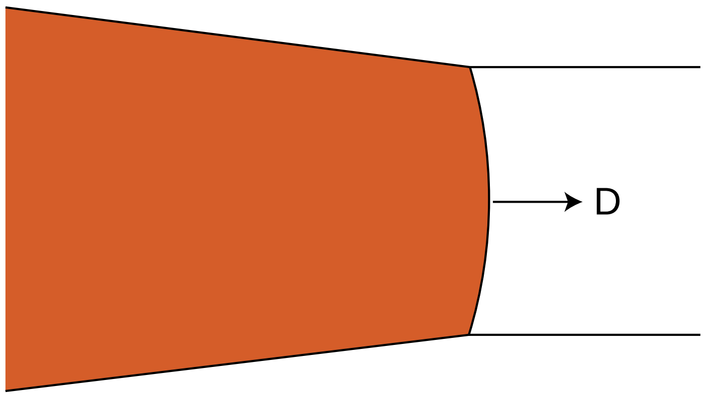

P
N
N_1
S
CJ
Rayleigh line
W
W_1
Fully reacted
Partially reacted
Unreacted
I
v
N_1
Subsonic
S
Supersonic
W_1
I
Pressure

Summary of steady, planar waves

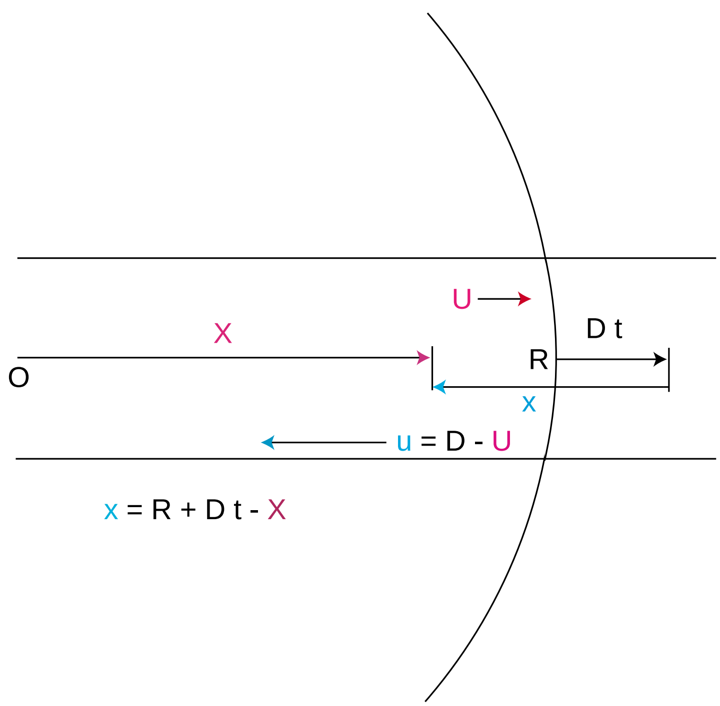
- Three kinds of steady structures are feasible: weak, hybrid and strong.
- Weak and hybrid structures require an initiation mechanism; hence not common in practice. However, they play an important role in the birth of a detonation.
- The strong structure is **ZND**: a lead shock anchoring a **fast flame**.
- For $D = D_{CJ}$ the exit state ($\lambda = 1$) is sonic.
- For $D > D_{CJ}$ the exit state is supersonic for a weak structure, and subsonic for hybrid and strong structures.
- Typically, an unsupported wave is a CJ wave, followed by a rarefaction.
- **Overdriven** waves ($D > D_{CJ}$, strong structure) require additional support (e.g., a piston).

Steady, Curved Waves in Slightly Divergent Flow

Observation



An approximate, 1-D model



Mass balance in cylindrical coordinates

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial X}(\rho U) = -\frac{\rho U}{X}$$

Coodinate transformation $(X, t) \Rightarrow (x, t)$

$$\frac{\partial}{\partial X} \Rightarrow -\frac{\partial}{\partial x}$$
$$\frac{\partial}{\partial t} \Rightarrow \frac{\partial}{\partial t} + D\frac{\partial}{\partial x}$$

Mass balance $\Rightarrow$

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + D\frac{\partial \rho}{\partial x} - \frac{\partial}{\partial x}(\rho U) &= -\frac{\rho U}{R + Dt - x} \\
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}[\rho(D - U)] &\approx -\frac{\rho U}{R} \\
\frac{\partial}{\partial x}(\rho u) &\approx -k\rho(D - u)
\end{aligned}$$

MODEL EQUATIONS FOR SLIGHTLY DIVERGENT FLOW

(Wave-fixed coordinates)

Upstream state: $p = 0,\ v = v_0,\ u = D$

Conservative Form

$$
\begin{aligned}
(\rho u)_x &= -\rho\alpha, \\
(p + \rho u^2)_x &= -\rho u \alpha, \\
\{(p + E\rho)u\}_x &= -(p + E\rho)\alpha, \\
(\rho u \lambda)_x &= \rho \mathcal{R} - \rho\lambda\alpha,
\end{aligned}
$$

Nonconservative Form

$$
\begin{aligned}
u\rho_x + \rho u_x &= -\rho\alpha, \\
\rho u u_x + p_x &= 0, \\
e_x + p v_x &= 0, \\
u\lambda_x &= \mathcal{R}.
\end{aligned}
$$

$$E = e + \frac{1}{2}u^2, \quad \alpha = k(D - u), \quad k = \text{ curvature.}$$

- **A full complement of algebraic conservation conditions is no longer available**
- **Structure problem now governed by an ODE system**

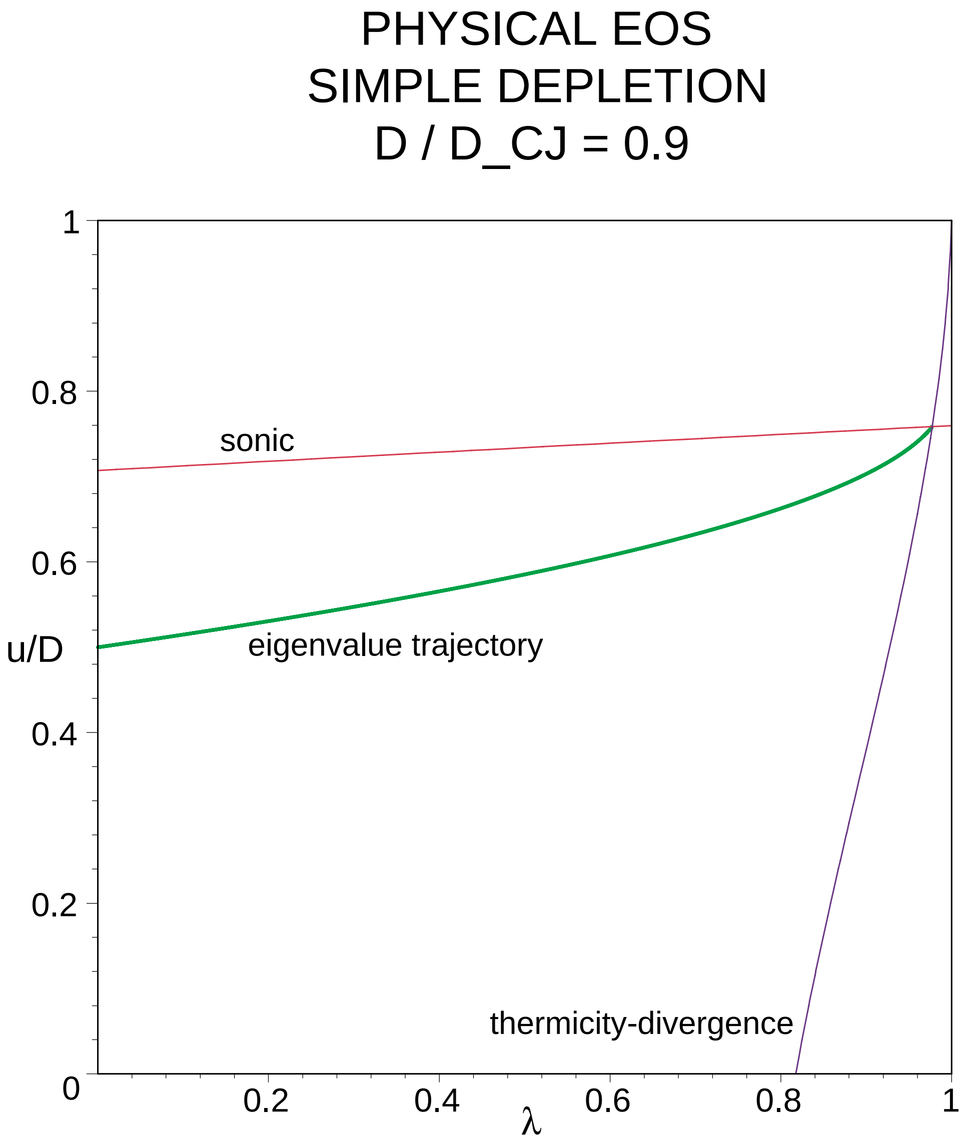
Equations Governing Reaction-Zone Structure

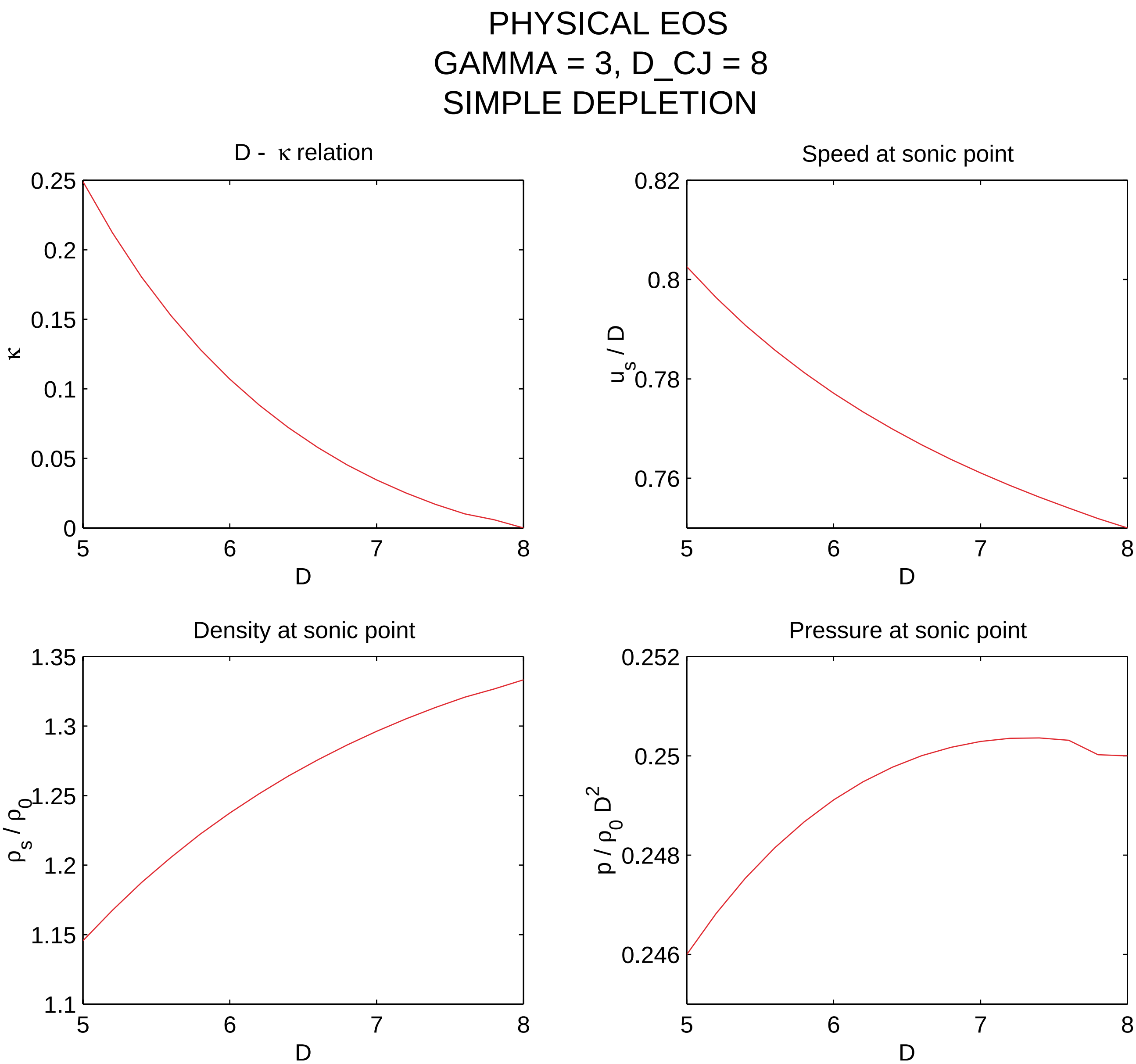
rate: $x \Longrightarrow \lambda$

$$
\begin{aligned}
e + pv &= \frac{\gamma p v}{\gamma - 1} - \lambda q \;=\; \frac{1}{2}(D^2 - u^2) \\
\frac{d(\rho u)}{d\lambda} &= -\rho u \frac{\alpha}{\mathcal{R}} \\
\frac{du}{d\lambda} &= \frac{[(\gamma - 1) q \mathcal{R} - c^2 \alpha] u}{(c^2 - u^2)\mathcal{R}}
\end{aligned}
$$

$$
\begin{aligned}
c^2 &= \frac{\gamma - 1}{2}(2\lambda q + D^2 - u^2) \\
\alpha &= k(D - u)
\end{aligned}
$$

- Divergence causes $\mathcal{R}$ to play a role in the structure.
- $\mathcal{R}(\lambda, T)$ is effectively a function of λ and u : hence structure analysis in the λu-plane is viable.
- Trajectories cross the sonic locus $\mathcal{S} \equiv c^2 - u^2 = 0$ vertically, and the thermicity-divergence locus $\mathcal{TD} \equiv (\gamma - 1) q \mathcal{R} - c^2 \alpha = 0$ horizontally.
- Smooth passage through the critical point $\mathcal{S} = \mathcal{TD} = 0$ requires a unique trajectory (eigenvalue detonation), on which $D = D(k)$.
- Asymptotic analysis for $k \to 0$ feasible.


PHYSICAL EOS
SIMPLE DEPLETION
D / D_CJ = 0.9
sonic
eigenvalue trajectory
thermicity-divergence
u/D
λ
0
0.2
0.4
0.6
0.8
1


PHYSICAL EOS
GAMMA = 3, D_CJ = 8
SIMPLE DEPLETION
D - κ relation
κ
0.25
0.2
0.15
0.1
0.05
0
5
6
7
8
D
Speed at sonic point
u_s / D
0.82
0.8
0.78
0.76
5
6
7
8
D
Density at sonic point
ρ_s / ρ_0
1.35
1.3
1.25
1.2
1.15
1.1
5
6
7
8
D
Pressure at sonic point
p / ρ_0 D^2
0.252
0.25
0.248
0.246
5
6
7
8
D

Status of the Simple Theory

- Steady structure is generally well-understood.
- Unsteady behavior less so and requires further work:
  - evolution from quiescent conditions upon stimulus (activation-energy asymptotics, Newtonian asymptotics)
  - transition from deflagration to detonation (DDT)
  - instabilities: development of cellular structures
  - propagation of front in complex geometry
  - failure to propagate

Implications of $T_a \gg 1$

Rate equation

$$\dot{\lambda} = k(1-\lambda)\exp(-T_a/T)$$

Scaled with respect to reference $(\lambda = 0,\ T = 1)$ state

$$\dot{\lambda} = (1-\lambda)\exp\left[T_a\left(1-\frac{1}{T}\right)\right]$$

$1 - \frac{1}{T} > 0$ and $O(1)$

Either reaction completed $(\lambda \sim 1)$ or gradients large

$1 - \frac{1}{T} < 0$ and $O(1)$

Rate is exponentially small; reaction frozen

$1 - \frac{1}{T} = o(1)$

$$1 - \frac{1}{T} = \frac{1}{T_a}\phi, \quad \text{rate} \ \sim \ (1-\lambda)e^{\phi}$$

Reaction confined to narrow zones of temperature and/or thin layers in space/time

Planar, One-dimensional Geometry

Lagrangian (mass-weighted) coordinate

$$\psi = \int_{x_0(t)}^{x} \rho(\xi, t)\, d\xi$$

$$\left.\frac{\partial F}{\partial x}\right)_t = \rho \left.\frac{\partial F}{\partial \psi}\right)_t, \qquad \left.\frac{\partial F}{\partial t}\right)_x + u \left.\frac{\partial F}{\partial x}\right)_t \equiv \dot{F} = \left.\frac{\partial F}{\partial t}\right)_\psi$$

<u>Reactive Euler Equations</u>

$$v_t - u_\psi = 0, \quad u_t + p_\psi = 0, \quad p_t + \frac{\gamma p}{v} v_t = (\gamma - 1) q \, \frac{\mathcal{R}}{v}, \quad \lambda_t = \mathcal{R}$$

$$T = \frac{pv}{R}, \quad \mathcal{R} = k(1 - \lambda) \exp(-T_a/T)$$

<u>Reference State</u>

$$p_0,\ v_0,\ T_0,\ c_0 = \sqrt{\gamma p_0 v_0}$$

$$t_0 = \frac{\epsilon}{k} \, \frac{c_p T_0}{q} \exp(T_a/T_0), \quad L_0 = c_0 t_0$$

$$\epsilon = T_0/T_a \ll 1 \ \ \text{(inverse activation energy)}$$

$$Q = \frac{\beta}{\gamma} = \frac{q}{c_p T_0} \quad \text{(heat-release parameter)}$$

<u>Dimensionless equations</u>

$$v_t - u_\psi = 0, \quad u_t + \frac{1}{\gamma}\, p_\psi = 0, \quad p_t + \frac{\gamma p}{v} v_t = \frac{\gamma \mathcal{R}}{v}, \quad \lambda_t = \frac{1}{Q}\mathcal{R}$$

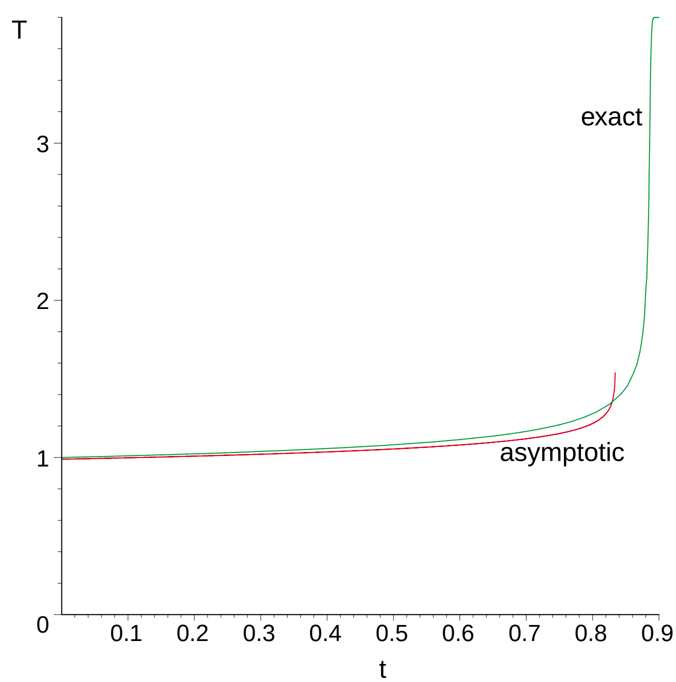
$$T = pv, \quad \mathcal{R} = \epsilon(1 - \lambda) \exp\left[\frac{1}{\epsilon}\left(1 - \frac{1}{T}\right)\right]$$

Spatially Uniform Evolution

$$u = 0, \quad v = 1, \quad p = T = 1 + \gamma Q \lambda.$$

$$T'(t) = \frac{\epsilon}{Q}(1 + \gamma Q - T) \exp\left[\frac{1}{\epsilon}\left(1 - \frac{1}{T}\right)\right], \quad T(0) = 1.$$

Evolution of temperature for ε = 1/14, Q = 2, γ = 1.4



In the limit $\epsilon \longrightarrow 0$,

$$T \sim 1 + \epsilon\phi(t), \quad \phi_t = \gamma e^{\phi}, \quad \phi(0) = 0, \quad \phi = -\ln(1 - \gamma t).$$

- Thermal runaway at $t_e \sim 1/\gamma$, onset of vigorous reaction.
- Following runaway, explosion proceeds with exponential rapidity, ending with $\lambda = 1$ and $T = 1 + \gamma Q$.
- Explosion time scale is σ, with $\gamma(t_e - t) = e^{-\sigma/\epsilon}$.

Spatially Uniform Evolution, contd.

- The more general initial condition

$$T(0) = 1 + \epsilon\phi_0$$

  produces runaway at

$$t_e \sim \frac{e^{-\phi_0}}{\gamma}.$$

  Order ϵ change in initial condition produces $O(1)$ change in induction time.

- Spatial nonuniformities (in temperature, or other gasdynamic variables) of $O(\epsilon)$ are likely to play an important role in the evolutionary process; such disturbances will have the ability to alter local induction times significantly, thereby introducing new physical phenomena in the induction process.